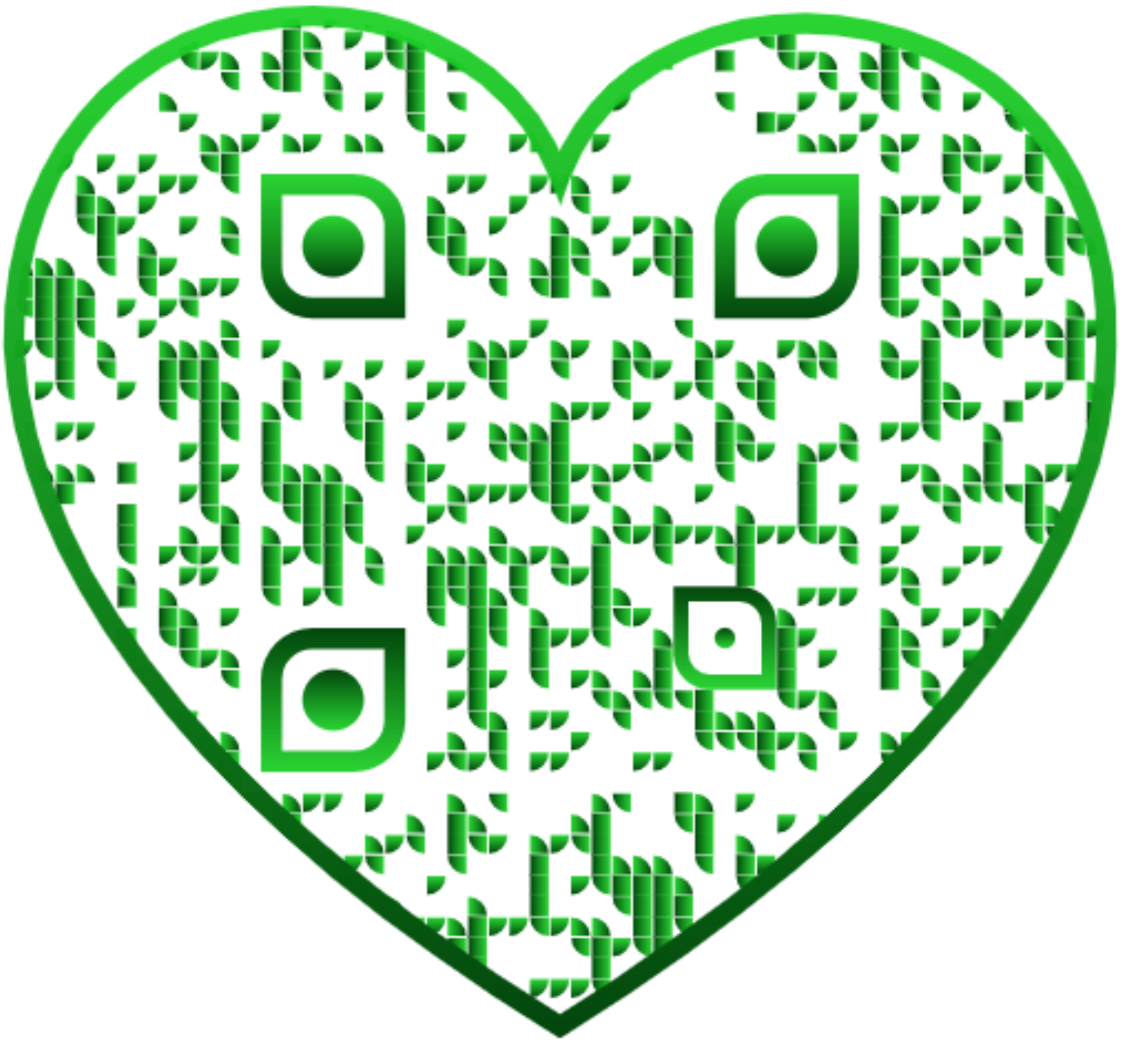
Chapter 3

Stoichiometry



Key skills

- Balance chemical equations
- Predict the products of simple combination, decomposition, and combustion reactions.
- Calculate formula weights
- Convert grams to moles and moles to grams using molar masses.
- Convert number of molecules to moles and moles to number of molecules using
  Avogadro's number
- Calculate the empirical and molecular formulas of a compound from percentage
  composition and molecular weight.
- Identify limiting reactants and calculate amounts, in grams or moles, or reactants
  consumed and products formed for a reaction.
- Calculate the percent yield of a reaction.

Introduction

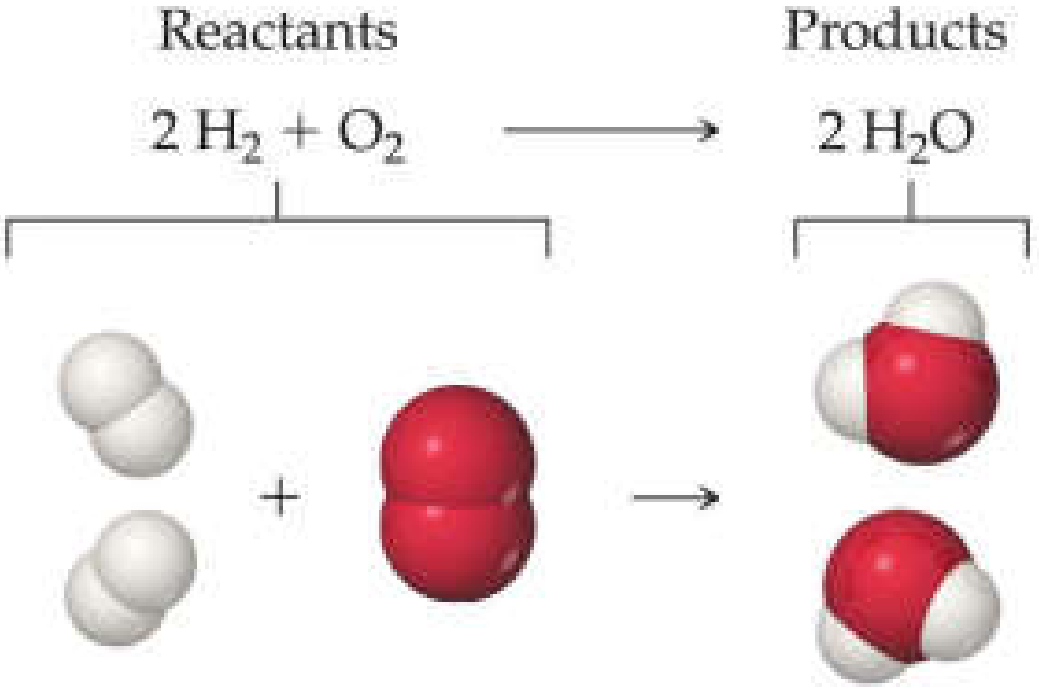
- **Stoichiometry** is the study of the *quantitative* relationships in substances and their reactions.
  - **Chemical equations**
  - **The mole and molar mass**
  - **Chemical formulas**
  - **Mass relationships in equations**
  - **Limiting reactant**

Definitions

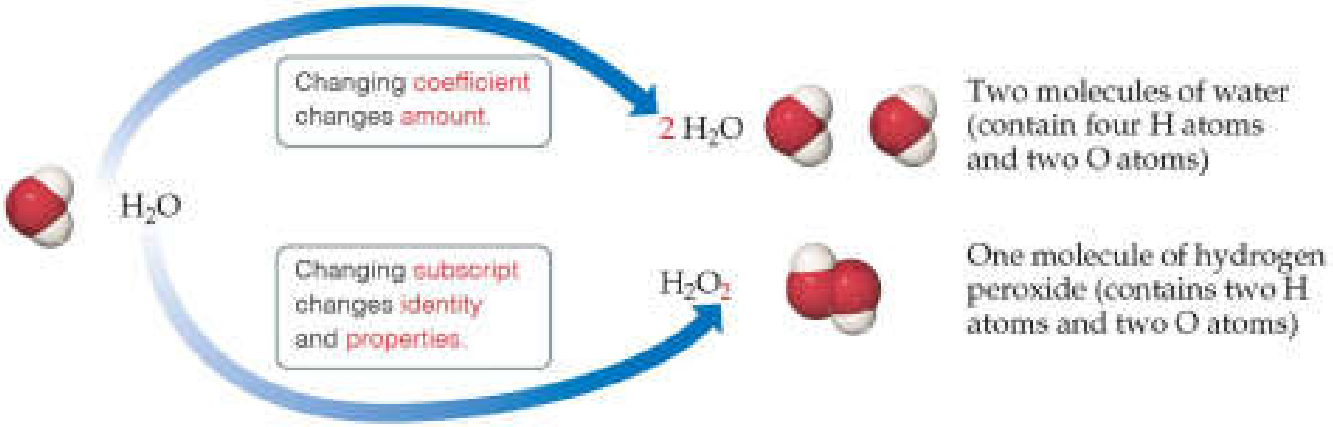
- **Reactants** are the substances consumed
- **Products** are the substances formed
- **Coefficients** are numbers before the formula of a substance in an equation
- A **balanced** equation has the same number of atoms of each element on both sides of the equation

Chemical Equations

- A chemical equation is a shorthand notation to describe a chemical reaction
  - Just like a chemical formula, a chemical equation expresses quantitative relations
- Subscripts tell the number of atoms of each element in a molecule
- Coefficients tell the number of molecules



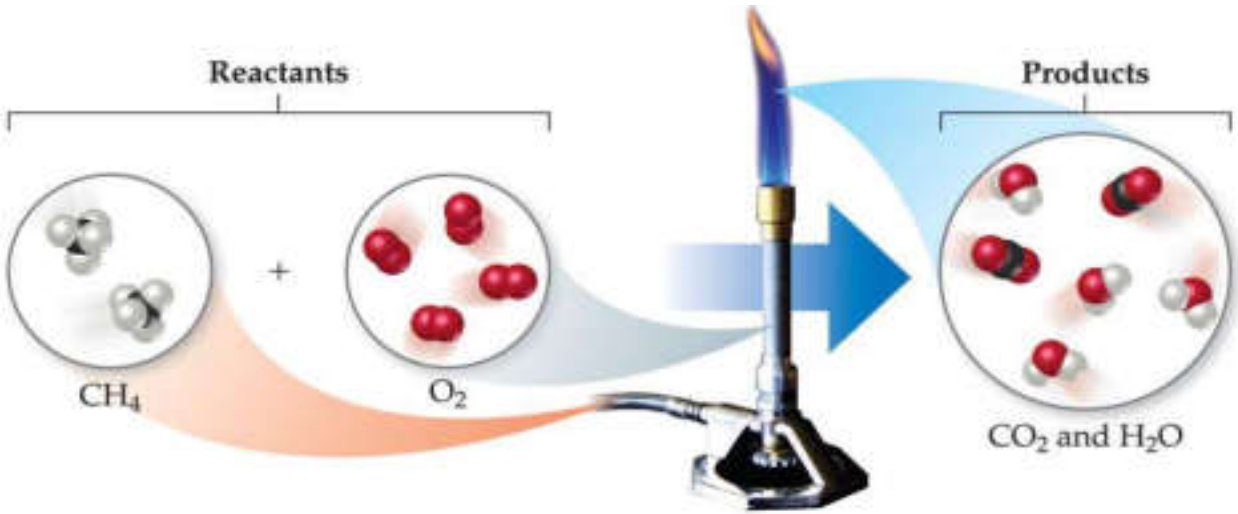
Coefficients vs. Subscripts


Changing coefficient changes amount.
2 H_2O
Two molecules of water (contain four H atoms and two O atoms)
H_2O
Changing subscript changes identity and properties.
H_2O_2
One molecule of hydrogen peroxide (contains two H atoms and two O atoms)

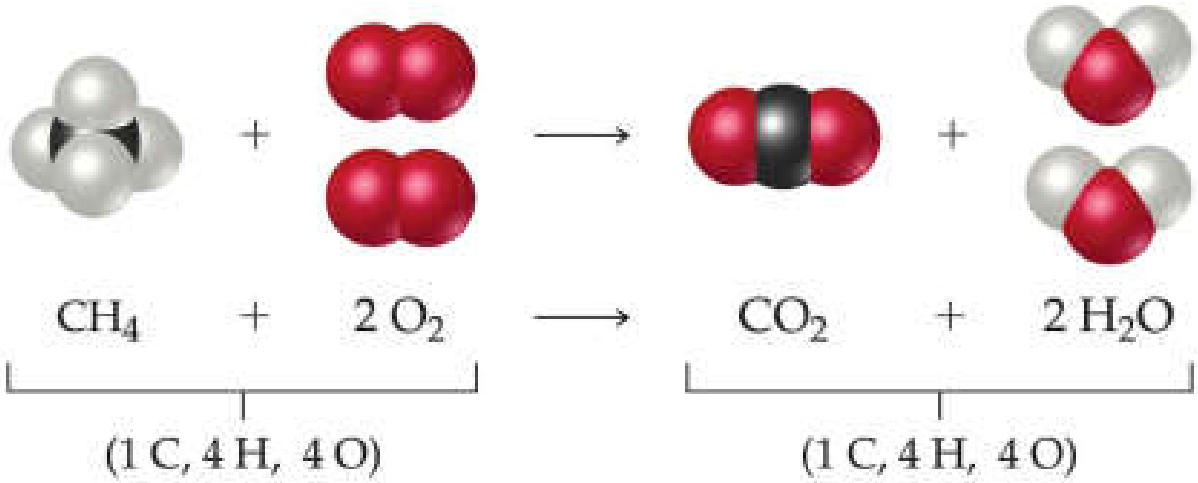
Hydrogen and oxygen can make water or hydrogen peroxide

$$2\ H_2(g) + O_2(g) \rightarrow 2\ H_2O(l)$$

$$H_2(g) + O_2(g) \rightarrow H_2O_2(l)$$



Anatomy of a Chemical Equation



Reactants appear on the left side of the equation.

Products appear on the right side of the equation.

The *states* of the reactants and products are written in parentheses to the right of each element symbol or formula.

Writing Balanced Equations

- Write the *correct formula* for each substance

  $H_2 + Cl_2 \rightarrow HCl$

- Add *coefficients* so the number of atoms of each element are the *same* on both sides of the equation

  $H_2 + Cl_2 \rightarrow 2HCl$

Balancing Chemical Equations

- Assume one molecule of the most complicated substance

  $C_5H_{12} + O_2 \rightarrow CO_2 + H_2O$

- Adjust the coefficient of CO_2 to balance C

  $C_5H_{12} + O_2 \rightarrow 5CO_2 + H_2O$

- Adjust the coefficient of H_2O to balance H

  $C_5H_{12} + O_2 \rightarrow 5CO_2 + 6H_2O$

- Adjust the coefficient of O_2 to balance O

  $C_5H_{12} + 8O_2 \rightarrow 5CO_2 + 6H_2O$

- Check the balance by counting the number of atoms of each element.

Balancing Equations

- Sometimes *fractional* coefficients are obtained

  $C_5H_{10} + O_2 \rightarrow CO_2 + H_2O$

  $C_5H_{10} + O_2 \rightarrow 5\ CO_2 + H_2O$

  $C_5H_{10} + O_2 \rightarrow 5\ CO_2 + 5\ H_2O$

  $C_5H_{10} + (15/2)\ O_2 \rightarrow 5\ CO_2 + 5\ H_2O$

- Multiply <u>all</u> coefficients by the denominator

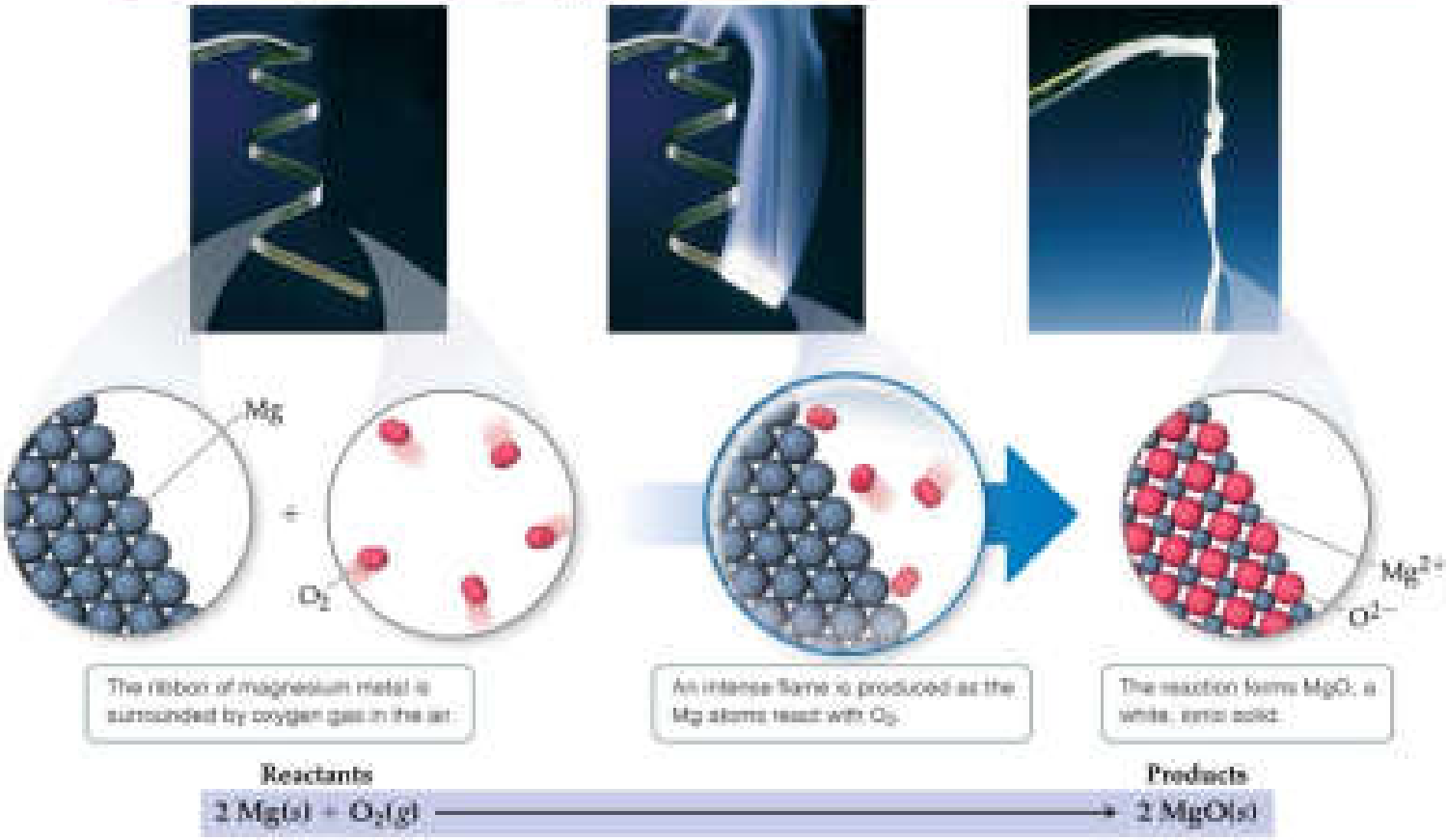
  $2\ C_5H_{10} + 15\ O_2 \rightarrow 10\ CO_2 + 10\ H_2O$

Combination

TABLE 3.1 Combination and Decomposition Reactions

Combination Reactions

$A + B \longrightarrow C$	Two or more reactants combine to form a single product. Many elements react with one another in this fashion to form compounds.
$C(s) + O_2(g) \longrightarrow CO_2(g)$	
$N_2(g) + 3H_2(g) \longrightarrow 2NH_3(g)$	
$CaO(s) + H_2O(l) \longrightarrow Ca(OH)_2(aq)$	


Mg
+
O_2
Mg^{2+}
O^{2-}
The ribbon of magnesium metal is surrounded by oxygen gas in the air.
An intense flame is produced as the Mg atoms react with O_2.
The reaction forms MgO, a white, ionic solid.
Reactants
Products
$2Mg(s) + O_2(g) \longrightarrow 2MgO(s)$

Decomposition

One substance breaks down into two or more substances

$2\ NaN_3\ (s) \longrightarrow 2\ Na\ (s) + 3\ N_2\ (g)$

$CaCO_3\ (s) \longrightarrow CaO\ (s) + CO_2\ (g)$

$2\ KClO_3\ (s) \longrightarrow 2\ KCl\ (s) + O_2\ (g)$

TABLE 3.1 Combination and Decomposition Reactions

Decomposition Reactions	
$C \longrightarrow A + B$	A single reactant breaks apart to form two or more substances. Many compounds react this way when heated.
$2\ KClO_3(s) \longrightarrow 2\ KCl(s) + 3\ O_2(g)$	
$PbCO_3(s) \longrightarrow PbO(s) + CO_2(g)$	
$Cu(OH)_2(s) \longrightarrow CuO(s) + H_2O(g)$	

Combustion

Is the process of burning, the combination of an organic substance with oxygen to produce a flame.

- When an organic compound burns in oxygen, the carbon reacts with oxygen to form CO_2, and the hydrogen forms water, H_2O.

Balance the following combustion reactions:

$$C_3H_8 + O_2 \rightarrow CO_2 + H_2O$$

$$(C_2H_5)_2O + O_2 \rightarrow CO_2 + H_2O$$

Formula Weight (FW)

- Sum of the atomic weights for the atoms in a chemical formula
- The formula weight of calcium chloride, $CaCl_2$, would be

Ca: 1(40.08 amu)
+ Cl: 2(35.45 amu)
110.98 amu

- Formula weights are generally reported for *ionic* compounds

Molecular Weight (MW)

- Sum of the atomic weights of the atoms in a molecule
- For the molecule ethane, C_2H_6, the molecular weight would be

C: 2(12.01 amu)
+ H: 6(1.008 amu)
30.07 amu

Percent Composition

• One can find the percentage of the mass of a compound that comes from each of the elements in the compound by using this equation:

$$\% \text{ element} = \frac{(\text{number of atoms})(\text{atomic weight})}{(\text{FW of the compound})} \times 100\%$$

Percent Composition

Example : the percentage by mass of carbon in ethane (C_2H_6) is

$$\%C = \frac{(2)(12.01\ \text{amu})}{(30.068\ \text{amu})} \times 100$$

$$= \frac{24.02\ \text{amu}}{30.068\ \text{amu}} \times 100$$

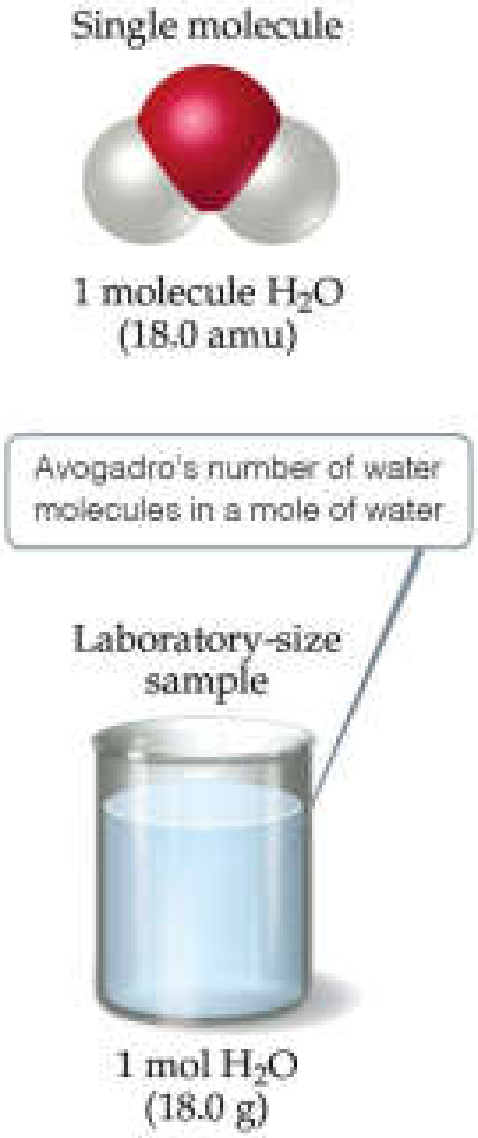
$$= 79.89\%$$

The Mole

- One **mole** is the amount of substance that contains as many entities as the number of atoms in exactly 12 grams of the ^{12}C isotope of carbon.
- **Avogadro's number** is the *experimentally determined* number of atoms in 12 g of isotopically pure ^{12}C, and is equal to 6.022×10^{23}
- One mole of anything contains 6.022×10^{23} entities
  - 1 mol H = 6.022×10^{23} atoms of H
  - 1 mol H_2 = 6.022×10^{23} molecules of H_2
  - 1 mol CH_4 = 6.022×10^{23} molecules of CH_4
  - 1 mol $CaCl_2$ = 6.022×10^{23} formula units of $CaCl_2$

Moles to Number of Entities

Moles of substance → (**Avogadro's number**) → **Number of atoms or molecules**



Example Calculations

- How many Na atoms are present in 0.35 mol of Na?
- How many moles of C_2H_6 are present in 3.00×10^{21} molecules of C_2H_6?

TABLE 3.2 Mole Relationships

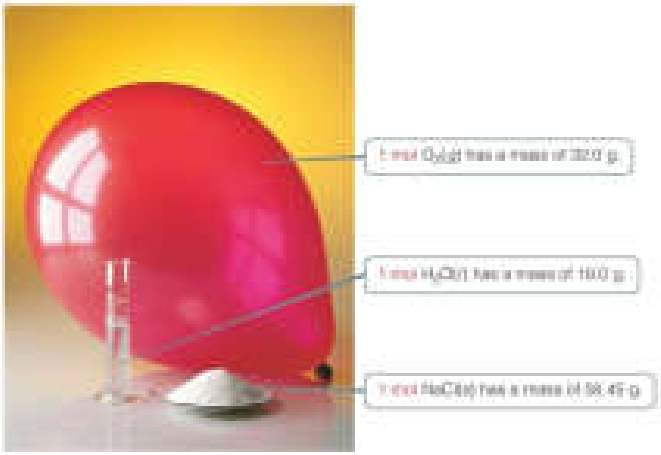
Name of Substance	Formula	Formula Weight (amu)	Molar Mass (g/mol)	Number and Kind of Particles in One Mole
Atomic nitrogen	N	14.0	14.0	6.02×10^{23} N atoms
Molecular nitrogen or "dinitrogen"	N_2	28.0	28.0	6.02×10^{23} N_2 molecules $2(6.02 \times 10^{23})$ N atoms
Silver	Ag	107.9	107.9	6.02×10^{23} Ag atoms
Silver ions	Ag^+	107.9[a]	107.9	6.02×10^{23} Ag^+ ions
Barium chloride	$BaCl_2$	208.2	208.2	6.02×10^{23} $BaCl_2$ formula units 6.02×10^{23} Ba^{2+} ions $2(6.02 \times 10^{23})$ Cl^- ions

[a]Recall that the mass of an electron is more than 1800 times smaller than the masses of the proton and the neutron; thus, ions and atoms have essentially the same mass.

Molar Mass

The **molar mass** ($\mathcal{M}$) of any atom, molecule or compound is the mass (in grams) of one mole of that substance.

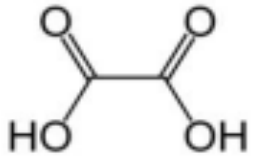
The molar mass *in grams* is numerically equal to the atomic mass or molecular mass expressed *in u (or amu)*.



Substance	Atomic Scale: Name	Atomic Scale: Mass	Lab Scale: Molar Mass
Ar	atomic mass	39.95 u	39.95 g/mol
C_2H_6	molecular mass	30.07 u	30.07 g/mol
NaF	formula mass	41.99 u	41.99 g/mol

Exercise 1

What mass of compound must be weighed out, to have a 0.0223 mol sample of $H_2C_2O_4$ ($\mathcal{M}$ = 90.04 g/mol)?



Oxalic acid

Interconverting masses and number of formula units

Example Calculation

What is the mass of 0.25 moles of CH_4?

$$0.25 \text{ mol } CH_4 \left(\frac{16.0 \text{ g } CH_4}{1 \text{ mol } CH_4} \right) = 4.0 \text{ g } CH_4$$

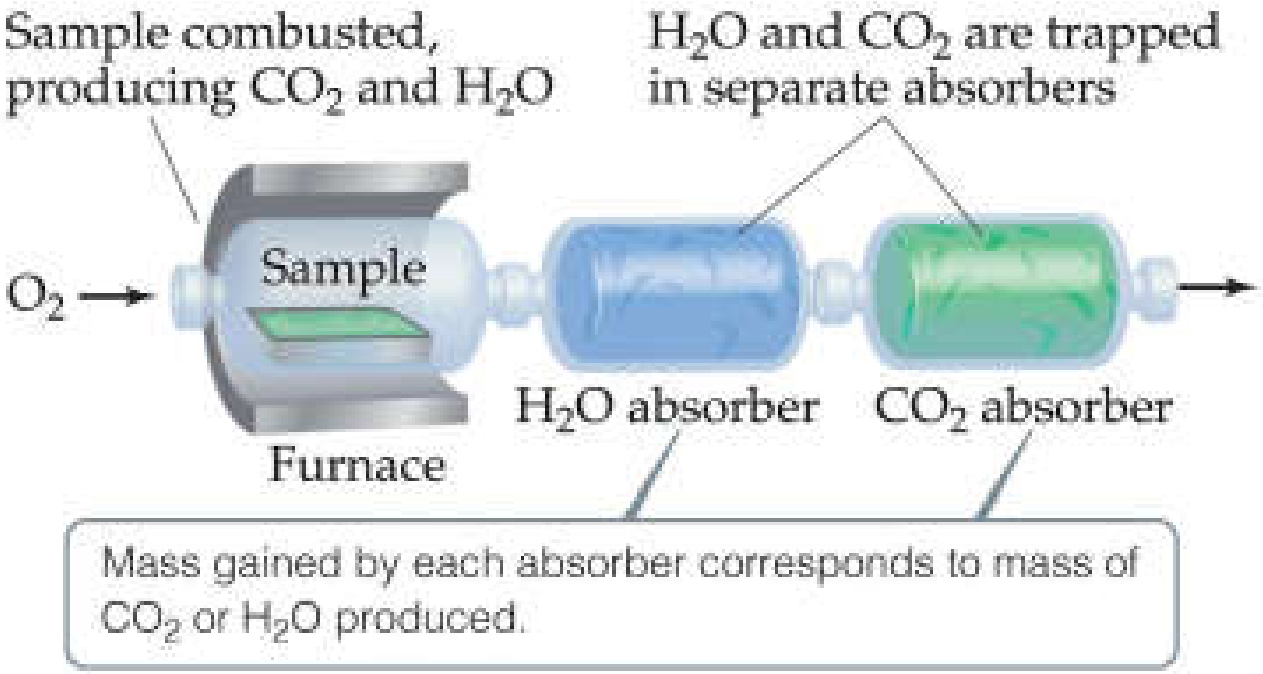
Empirical formula

Exercise 2

Example 1: What is the empirical formula of a compound that contains 0.799 g C and 0.201 g H in a 1.000 g sample?

Example 2: What is the empirical formula of a chromium oxide that is 68.4% Cr by mass?

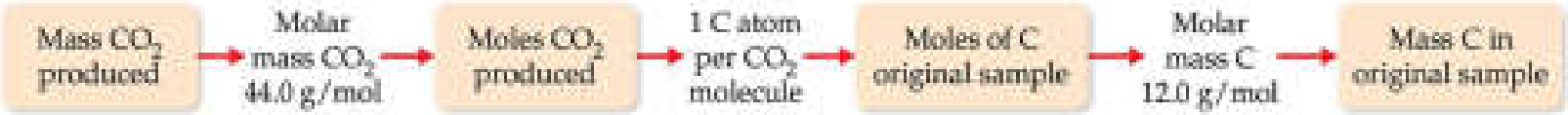
Combustion Analysis


Sample combusted, producing CO_2 and H_2O
H_2O and CO_2 are trapped in separate absorbers
O_2
Sample
Furnace
H_2O absorber
CO_2 absorber
Mass gained by each absorber corresponds to mass of CO_2 or H_2O produced.

- Compounds containing C, H and O are routinely analyzed through combustion in a chamber like this
  - C is determined from the mass of CO_2 produced
  - H is determined from the mass of H_2O produced
  - O is determined by difference after the C and H have been determined

Finding C and H content

- A weighed sample of compound is burned, and the masses of H_2O and CO_2 formed is measured.


Mass CO_2 produced
Molar mass CO_2 44.0 g/mol
Moles CO_2 produced
1 C atom per CO_2 molecule
Moles of C original sample
Molar mass C 12.0 g/mol
Mass C in original sample

Mass H_2O produced
Molar mass H_2O 18.0 g/mol
Moles H_2O produced
2 H atoms per H_2O molecule
Moles H in original sample
Molar mass H 1.01 g/mol
Mass H in original sample

Calculating Empirical Formulas

- **Example 1:** The compound *para*-aminobenzoic acid (you may have seen it listed as PABA on your bottle of sunscreen) is composed of carbon (**61.31%**), hydrogen (**5.14%**), nitrogen (**10.21%**), and oxygen (**23.33%**). Find the empirical formula of PABA.

Assuming 100.00 g of *para*-aminobenzoic acid,

$$\text{C:} \quad 61.31\ \text{g} \times \frac{1\ \text{mol}}{12.01\ \text{g}} = 5.105\ \text{mol C}$$

$$\text{H:} \quad 5.14\ \text{g} \times \frac{1\ \text{mol}}{1.01\ \text{g}} = 5.09\ \text{mol H}$$

$$\text{N:} \quad 10.21\ \text{g} \times \frac{1\ \text{mol}}{14.01\ \text{g}} = 0.7288\ \text{mol N}$$

$$\text{O:} \quad 23.33\ \text{g} \times \frac{1\ \text{mol}}{16.00\ \text{g}} = 1.456\ \text{mol O}$$

Example 2: Calculate the mole ratio by dividing by the smallest number of moles:

$$\text{C:} \quad \frac{5.105\ \cancel{\text{mol}}}{0.7288\ \cancel{\text{mol}}} = 7.005 \approx 7$$

$$\text{H:} \quad \frac{5.09\ \cancel{\text{mol}}}{0.7288\ \cancel{\text{mol}}} = 6.984 \approx 7$$

$$\text{N:} \quad \frac{0.7288\ \cancel{\text{mol}}}{0.7288\ \cancel{\text{mol}}} = 1.000$$

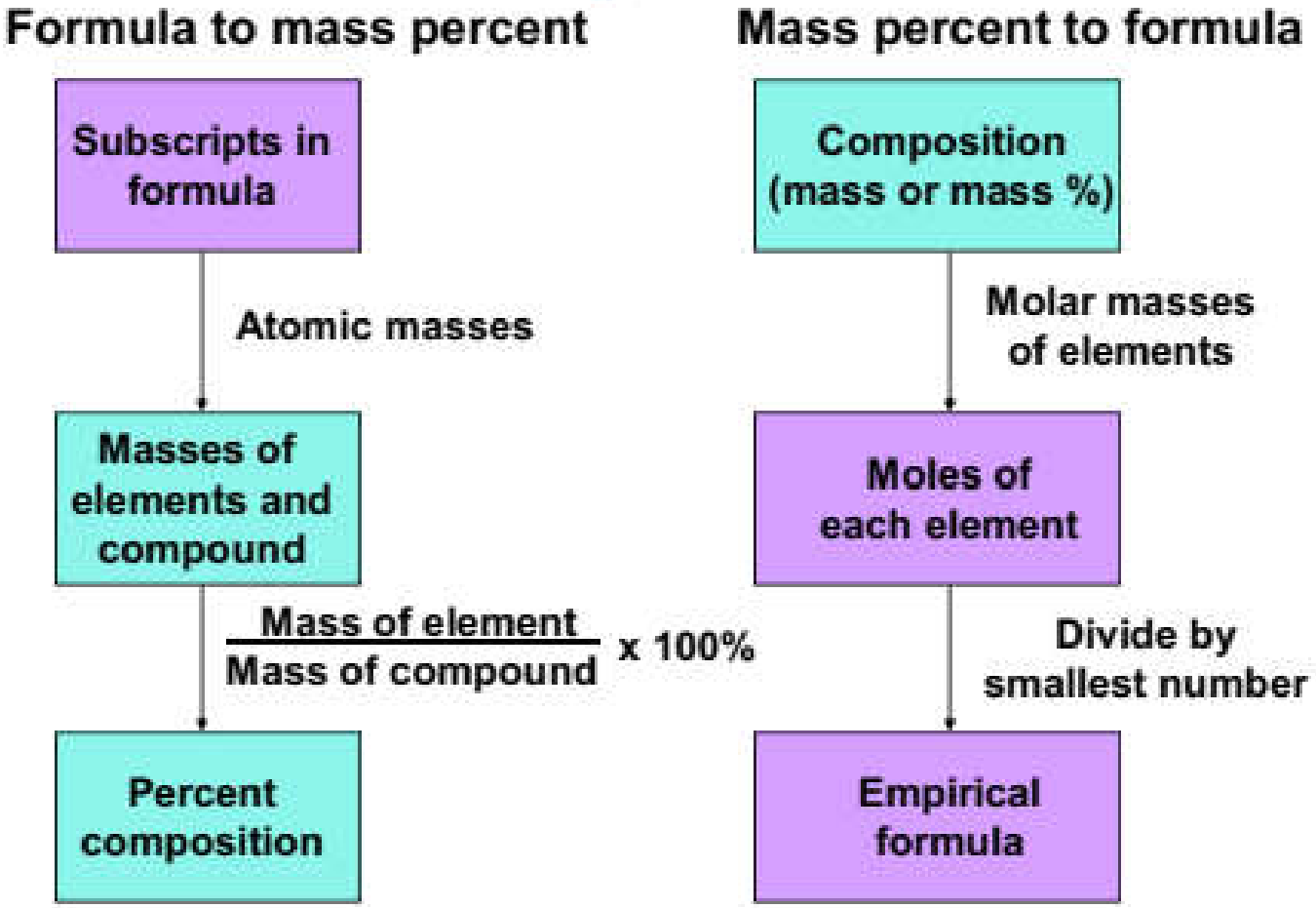
$$\text{O:} \quad \frac{1.458\ \cancel{\text{mol}}}{0.7288\ \cancel{\text{mol}}} = 2.001 \approx 2$$

$C_7H_7NO_2$

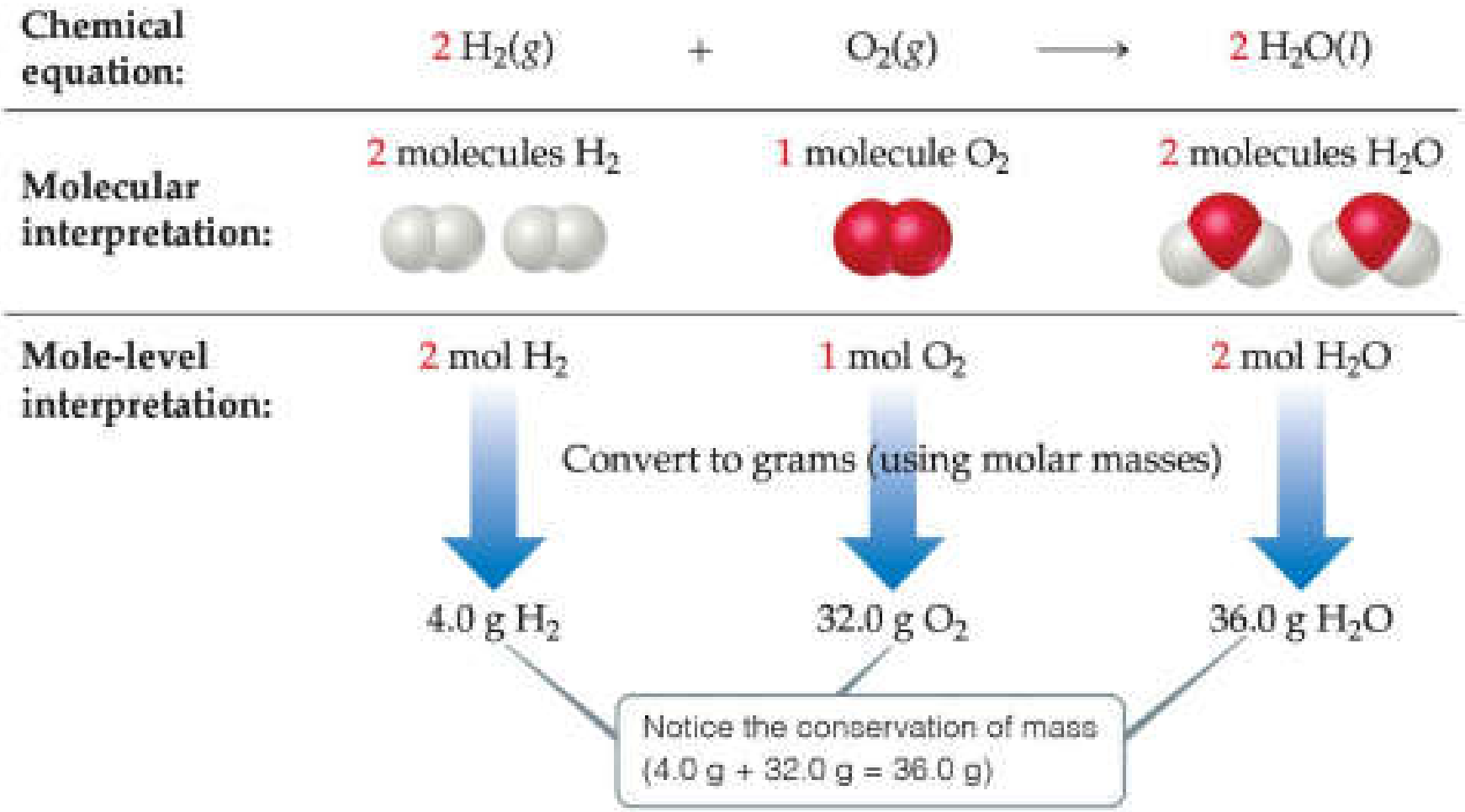
Exercise 3

1. A compound contains only C, H, and O. A 0.1000 g sample burns completely in oxygen to form 0.0930 g water and 0.2271 g CO_2. Calculate the mass of each element in this sample. What is the empirical formula of the compound?

Comparison


Formula to mass percent
Subscripts in formula
Atomic masses
Masses of elements and compound
Mass of element / Mass of compound x 100%
Percent composition
Mass percent to formula
Composition (mass or mass %)
Molar masses of elements
Moles of each element
Divide by smallest number
Empirical formula

Mole Relationships in Equations



Guidelines for Reaction Stoichiometry

- Write the balanced equation.
- Calculate the number of moles of the species for which the mass is given.
- Use the coefficients in the equation to convert the moles of the given substance into moles of the substance desired.
- Calculate the mass of the desired species.

Exercise 4

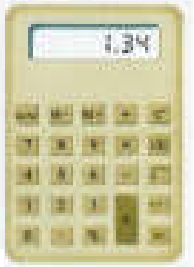
1. Given the reaction $4FeS_2 + 11\ O_2 \rightarrow 2Fe_2O_3 + 8SO_2$

What mass of SO_2 is produced from reaction of 3.8 g of FeS_2 and excess O_2?

2. What mass of SO_3 forms from the reaction of 4.1 g of SO_2 with an excess of O_2?

Reaction Yields

Actual yield is found by measuring the quantity of product formed in the experiment.



Theoretical yield is calculated from reaction stoichiometry.

$$\% \text{ yield} = \frac{\text{Actual yield}}{\text{Theoretical yield}} \times 100\%$$

Example: Calculating Percent Yield

A 10.0 g-sample of potassium bromide is treated with perchloric acid solution. The reaction mixture is cooled and solid $KClO_4$ is removed by filtering, then it is dried and weighed.

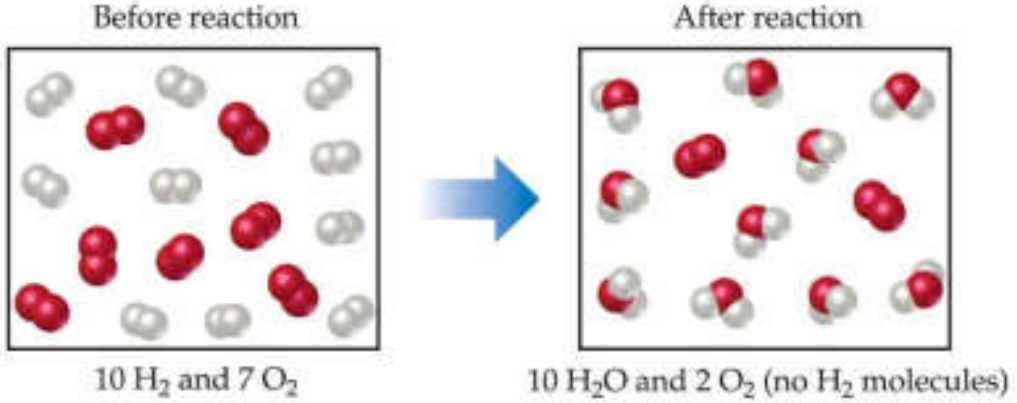
$$KBr\,(aq) + HClO_4\,(aq) \rightarrow KClO_4\,(s) + HBr\,(aq)$$

The product weighed 8.8 g. What was the percent yield?

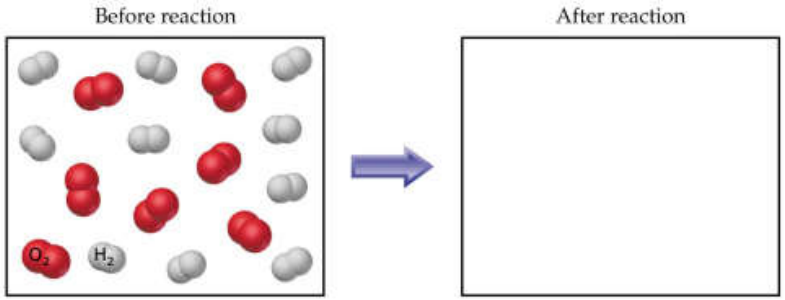
Limiting Reactant

Limiting reactant : the reactant that is completely consumed in a reaction. When it is used up, the reaction stops, thus limiting the quantities of products formed.

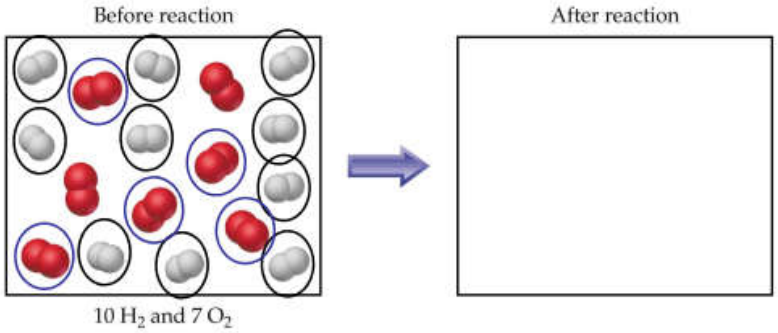
Excess reactant : the other reactants present, not completely consumed



$$2H_2(g) + O_2(g) \rightarrow 2H_2O(g)$$

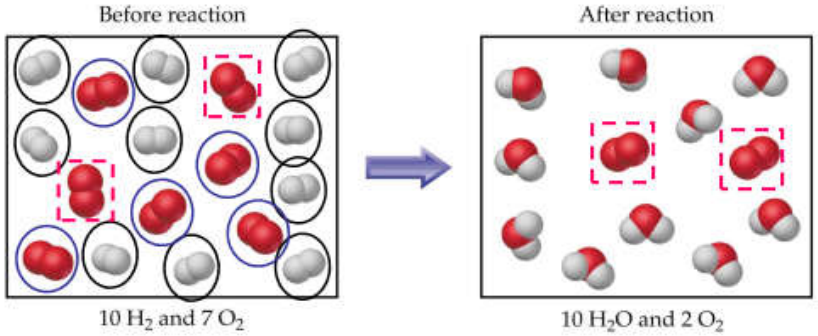


$$2H_2(g) + O_2(g) \rightarrow 2H_2O(g)$$



$$\mathbf{5[2H_2(g) + O_2(g) \rightarrow 2H_2O(g)]}$$
$$\mathbf{10H_2(g) + 5O_2(g) \rightarrow 10H_2O(g)}$$

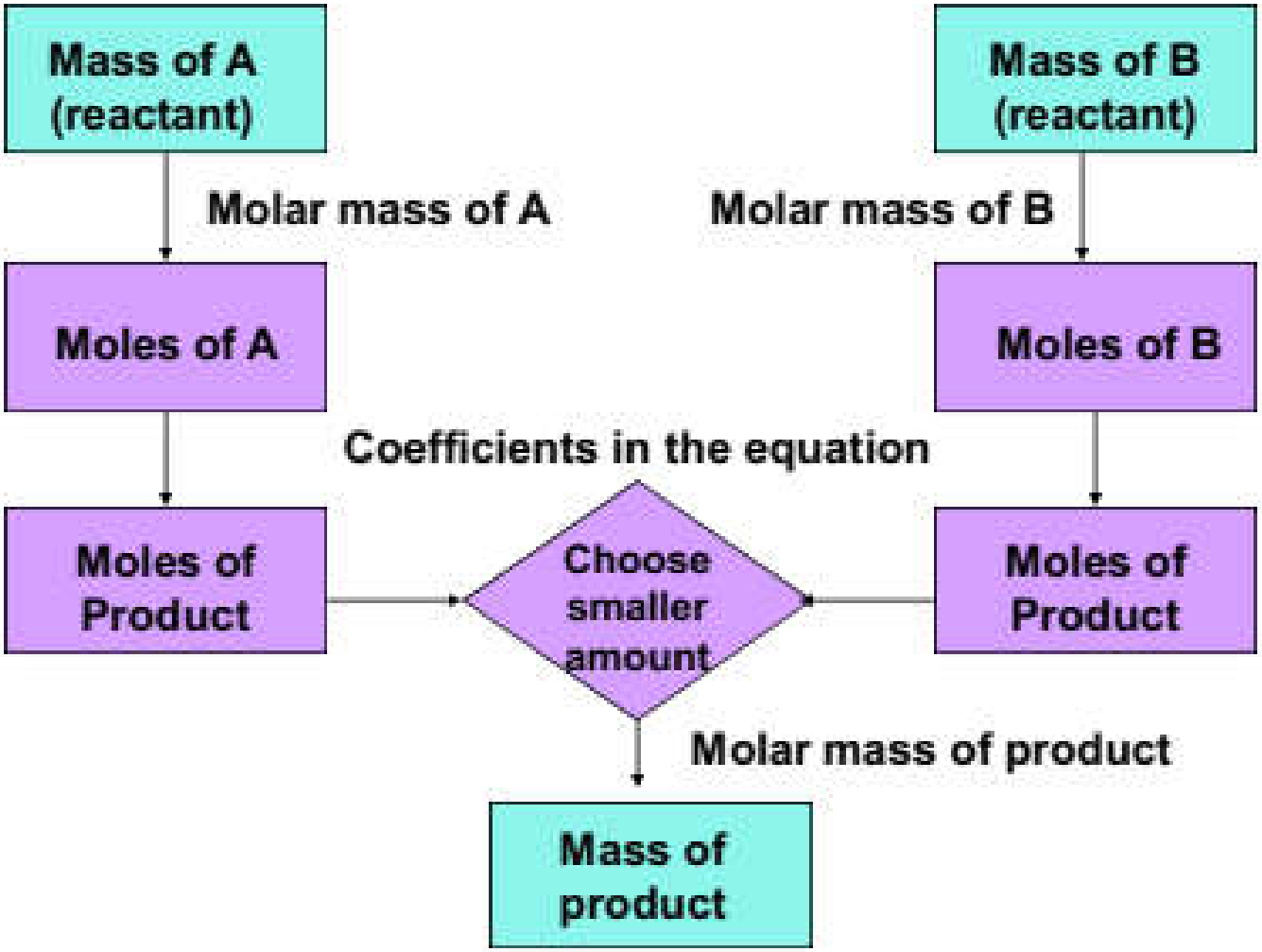
$$2H_2(g) + O_2(g) \rightarrow 2H_2O(g)$$



$$\mathbf{5[2H_2(g) + O_2(g) \rightarrow 2H_2O(g)]}$$
$$\mathbf{10H_2(g) + 5O_2(g) \rightarrow 10H_2O(g)}$$

	$2\,H_2(g)$	+	$O_2(g)$	$\longrightarrow$	$2\,H_2O(g)$
Before reaction:	10 mol		7 mol		0 mol
Change (reaction):	−10 mol		−5 mol		+10 mol
After reaction:	0 mol		2 mol		10 mol

Strategy for Limiting Reactant



Exercise 5

1. Calculate the theoretical yield (g) when 7.0 g of N_2 reacts with 2.0 g of H_2, forming NH_3.

2. One reaction step in the conversion of ammonia to nitric acid involves converting NH3 to NO by the following reaction:

$$4\ NH_3(g) + 5\ O_2(g) \rightarrow 4\ NO(g) + 6\ H_2O(g)$$

- If 1.50 g of NH_3 reacts with 2.75 g O_2, then:

a. Which is the limiting reactant?

b. How many grams of NO and H_2O form?

c. How many grams of the excess reactant remain after the limiting reactant is completely consumed?

d. Is the law of conservation of mass obeyed?